Technical Data Sheet
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DIBAH
Diisobutylaluminum hydride

CAS Number	1191-15-7
EINECS/EC	214-729-9
Molecular Formula	$(i\text{-}C_4H_9)_2AlH$

APPLICATION

Diisobutylaluminum hydride (DIBAH) is an excellent reducing agent, finding use in pharmaceutical, flavor, fragrance and other fine chemical processes requiring an active hydrogen reducing agent. Most applications involve reduction of carbonyl functionalities to alcohols or aldehydes and nitrogen functionalities to amines. DIBAH is soluble in aliphatic and aromatic hydrocarbons, as well as ether-type solvents.

SPECIFICATION

Aluminum, wt. %, min	18.5
DIBAH, wt. %, min	95.0
TEA, wt. %, max	0.5
TNPA, wt. %, max	1.5
TNBA, wt. %, max	0.6
TIBA, wt. %, max	5.5

DENSITY & VISCOSITY

Temperature		Density		Viscosity
°C	°F	g/mL	lbs/gal	cp
0	32	0.8162	6.81	35
10	50	0.8093	6.753	23.1
20	68	0.8024	6.695	16
25	77	0.7989	6.666	13.5
30	86	0.7954	6.638	11.5
40	104	0.7885	6.58	8.52
50	122	0.7816	6.522	6.5
60	140	0.7747	6.464	5.08
70	158	0.7678	6.407	4.05
80	176	0.7609	6.349	3.29
90	194	0.754	6.292	2.72
100	212	0.7471	6.234	2.28
120	248	0.7333	6.118	1.66
140	284	0.7194	6.003	1.26
160	320	0.7056	5.888	0.99
180	356	0.6918	5.773	0.8
200	392	0.678	5.657	0.66

Equations:

Density: d(g/mL) = 0.8162 - 0.000691t; t = °C

Viscosity: $\log_{10}(cp) = -1.5996 + 51\,8.66/(t + 165)$; t = °C

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PHYSICAL PROPERTIES

Property	Value
Formula	$(i\text{-}C4H_9)_2AlH$
Formula weight	142.22
State and color at 25°C	clear, colorless liquid
Stability in contact with air	flames instantly
Stability in contact with water	reacts violently
Melting point, °C (°F)	-80 (-112)
Boiling point at 760 mm Hg, °C (°F)	269.4 (516.9)
Vapor pressure at 20°C (68°F), mm Hg	0.000174
Vapor pressure at 40°C (104°F), mm Hg	0.0017
Vapor pressure at 60°C (140°F), mm Hg	0.01212
Vapor pressure at 80°C (176°F), mm Hg	0.0667
Vapor pressure at 100°C (212°F), mm Hg	0.2986
Vapor pressure at 120°C (248°F), mm Hg	1.132
Vapor pressure at 140°C (284°F), mm Hg	3.689
Vapor pressure at 160°C (320°F), mm Hg	10.513
Vapor pressure at 180°C (356°F), mm Hg	26.937
Vapor pressure at 200°C (392°F), mm Hg	63.358
Vapor pressure at 220°C (428°F), mm Hg	139.80
Vapor pressure at 240°C (464°F), mm Hg	286.98
Specific heat at 20°C, cal/g°C	0.489
Specific heat at 68°F, btu/lb°F	0.489
Heat of vaporization at NBP, cal/g	69.8
Heat of vaporization at NBP, btu/lb	125.7
ΔH of formation at 25°C, kcal/gfw	-62.8
Heat of combustion, net at 25°C, cal/g	10118
Heat of combustion, net at 77°F, btu/lb	18213
Heat of reaction with water at 25°C, cal/g	714
Heat of reaction with water at 77°F, btu/lb	1286
Coefficient of volume expansion at 25°C, per °C	0.000884
Critical pressure, atm	39.4
Critical temperature, °C	467.6
Decomposition rate at 100°C (%/min)	0.000331
Decomposition rate at 120°C (%/min)	0.000281
Decomposition rate at 140°C (%/min)	0.00112
Decomposition rate at 160°C (%/min)	0.00555
Decomposition rate at 180°C (%/min)	0.0240
Decomposition rate at 200°C (%/min)	0.0922
Decomposition rate at 240°C (%/min)	3.1900

HANDLING & STORAGE

The pyrophoric nature of DIBAH presents potential hazards not common to most liquid chemicals used by industry in tank truck quantities. DIBAH, being pyrophoric, breaks into flame spontaneously and gives off dense smoke when exposed to air. It reacts violently with water. DIBAH is a clear, non-corrosive mobile liquid with a low vapor pressure. Hydrocarbon solutions of DIBAH, depending on the concentration and temperature, may not be pyrophoric. However, these solutions must still be blanketed with an inert gas such as dry nitrogen because DIBAH will react with air and moisture at the surface of the solution, giving off dense smoke, heat and flammable gas. For specific information on the safe handling and toxicity of this product, please refer to the Material Safety Data Sheet, which is available upon request.

TRANSPORT & PACKAGING

	Nominal Value		Approximate Loadings	
Container Description	Gallons	Liters	Pounds	Kilograms
Tank Car (DOT-105A300W)	23,000-25,100	87,100-95,000	135,000-230,000	61,400- 104,000
Tank Trailer (DOT-MC330 or 331)	6,200-7,200	23,500-27,200	30,00-48,000	13,600- 21,800
Portable Tanks (DOT-51)/UN T21	430	1,635	2,250-3,800	1,021-1,725
	1,980	7,500	10,257-17,000	4,880-7,711
Isotank	5,635-5,970	21,330-22,600	30,000-34,000	13,600- 15,500
Cylinders: dual valve (DOT-4BA240)				
5 gallon size	5.7	22	25-53	11-24
26 gallon size	28.0	106	150-268	68-120
Laboratory cylinders (DOT-3AA2015)				
0.4 gallon size	0.40	1.47	1.2-2.2	0.58-0.97
1.0 gallon size	0.94	3.60	2.9-6.3	1.4-2.8

*Actual weight depends on highway load limits, product density and lifting considerations.

Shipments are made in accordance with DOT regulations — Section 173.134. All containers are shipped blanketed with dry nitrogen under slight positive pressure. Hydrocarbon solutions are also available blended to customer specifications.Tank rail cars and tank trucks are available in North America only.

Transportation Classification

Proper shipping name ..... Organometallic Substance, Liquid, Pyrophoric, Water Reactive (Diisobutylaluminum hydride)

Hazard class ..... 4.2 (spontaneously combustible) + 4.3(dangerous when wet)

ID number UN3394

Placard(s ..... spontaneously combustible w/ number 4+dangerous when wet 4

Label(s ..... spontaneously combustible+dangerous when wet

MARPOL Classification ..... n/a

Harmonized tariff number 2931.00.4000-2

Schedule B number 2931.00.6000-7

OTHER INFORMATION

Further Related Documents — Safety Data Sheet

The information presented herein is believed to be accurate and reliable, but is presented without guarantee or responsibility on the part of Albemarle Corporation and its subsidiaries and affiliates. It is the responsibility of the user to comply with all applicable laws and regulations and to provide for a safe workplace. The user should consider any health or safety hazards or information contained herein only as a guide, and should take those precautions which are necessary or prudent to instruct employees and to develop work practice procedures in order to promote a safe work environment. Further, nothing contained herein shall be taken as an inducement or recommendation to manufacture or use any of the herein materials or processes in violation of existing or future patent.

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